Ca/Cu process is essentially the numerical schemes adopted to solve the governing equations.

Future steps regarding the modelling part will be focused on the understanding of the system behaviour under different conditions and the integration in comprehensive process models.

ASCENT consortium

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Newsletter 27 March 2017 – Modelling in ASCENT and its experimental validation

The Ca/Cu looping process for H_2 production under development in the ASCENT project makes use of a Cu/CuO chemical loop to capture the CO_2 during the production of H_2 by sorption-enhanced reforming (SER) of CH_4 and supply the energy required for the endothermic $CaCO_3$ calcination via a chemical looping process. Currently some of the modelling activities are focused on the definition of the reactor models to simulate this process.

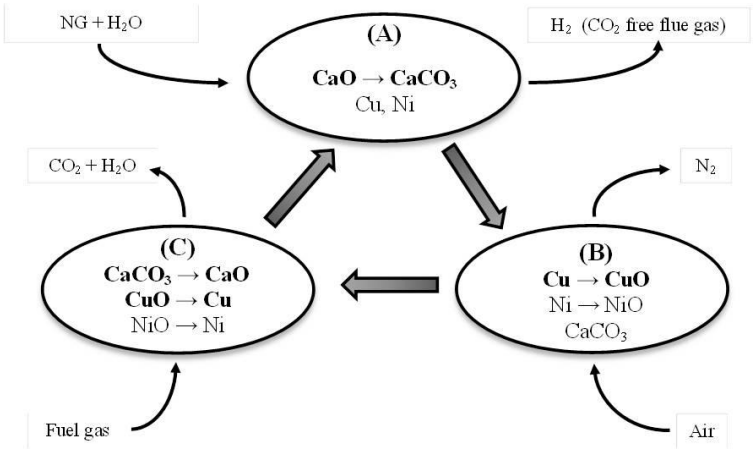

Figure 1 General scheme of the Ca/Cu three step chemical loop.

Two one-dimensional pseudo-homogeneous models are now available to describe this process: one solved in Delphi developed at Eindhoven University of Technology (TU/e) and one solved in Matlab developed at the *Instituto Nacional del Carbón* (INCAR) of *Consejo Superior de Investigaciones Científicas* (CSIC) in Oviedo. The two models have been compared with experimental results and have been compared with each other. Both models are able to capture the most important phenomena occurring during the Ca/Cu cycle. These two models will be used to design the experimental campaign in the available setups for the proof of concept in the TU/e laboratory.

Figure 2 Packed bed reactor setup at TU/e lab

Delphi model developed by TU/e – A fixed bed reactor model has been developed with a one-dimensional adiabatic pseudo-homogeneous model (PHM), using a finite difference technique with higher order discretization schemes and automatic grid and time step adaptation. This dynamic model simulates unsteady state processes accounting for axial mass and heat dispersion and convection and reaction kinetics, considering both gaseous and solid components. Steam methane reforming and water gas shift are heterogeneously catalyzed gas phase reactions over a nickel catalyst. The kinetics of these reactions have been extensively studied in the literature (i.e. Xu and Froment model and Numaguchi and Kikuchi model). Both kinetics have been implemented in the model. The carbonation of calcium oxide and subsequent calcination of calcium carbonate are described using the shrinking core model (SCM). Limestone kinetics were taken from

previous works developed in the ASCENT project. The experimental validation of the Ca-Cu process has been carried out in an existing facility at the TU/e laboratory with a previous campaign done in this project.

Matlab model developed by INCAR-CSIC - A one-dimensional pseudo-homogenous model has been developed to describe the different steps of the Ca-Cu process carried out in adiabatic fixed-bed reactors.

Figure 3 Experimental set up built at INCAR-CSIC.

The main assumptions here adopted are: mass and thermal dispersion in the axial direction, the absence of radial temperature or concentration gradients, negligible intra-particle concentration and temperature gradients at the scale of millimetres, ideal gas behaviour, a constant bed void fraction, perfect mixing of the solids, and a uniform particle size. All the physical properties were considered variable with temperature and composition. An experimental set up has been specifically constructed at INCAR-CSIC to study the CuO reduction/$CaCO_3$ calcination and the oxidation of Cu in a pseudo-adiabatic fixed-bed reactor. The dynamic reactor model described above has been partially validated with the experimental results gathered in this test-rig. The main difference between the two models developed for